Autonomic Subgrid-Scale Closure for Large Eddy Simulations

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Motivated by advances in PDE-constrained optimization, a fundamentally new autonomic closure for large eddy simulations (LES) is presented that implements an optimization formulation for the subgrid-scale stresses instead of using a predefined turbulence model. The autonomic closure approach is based on the most general dimensionally-consistent polynomial expansion of the local subgrid-scale stress tensor in terms of the resolved scale primitive variables and their products at all spatial locations and times. In so doing, the closure approach inherently addresses nonlinear, nonlocal, and nonequilibrium turbulence effects without introducing any tuning parameters. The expansion introduces a large set of coefficients that can be determined by solving an inverse problem that minimizes error relative to known subgrid stresses at a test filter scale. The resulting optimized coefficients are then projected to the LES scale by invoking scale similarity in the inertial range and applying appropriate renormalizations. This new closure approach avoids the need to specify a subgrid-scale model, and instead allows the optimization procedure to determine the best local relation between subgrid stresses and resolved-scale variables. Here we present the most general formulation of this new autonomic approach, and also present an inverse approach for determining the optimal coefficients. We then explore truncation, regularization, and sampling within the inverse formulation. Finally, we present results from a priori tests of the autonomic closure approach using data from direct numerical simulations of homogeneous isotropic and sheared turbulence. Even for the simplest 2nd order truncation of the fundamental polynomial expansion, substantial improvements over the Dynamic Smagorinsky model are found from this new autonomic closure approach.

I. Introduction

Turbulent flows of engineering and scientific importance typically involve an enormous range of spatial and temporal scales. The computational cost of resolving this full scale range is prohibitive for most applications, so large eddy simulations (LES) that coarse-grain the Navier-Stokes equations via low-pass filtering are commonly used to reduce the scale range that must be resolved. This coarsening results in a subfilter-scale stress tensor, \( \tau_{ij}(x, t) \), that must be modeled to account for the effects of subfilter scales on the filtered scales. Typically, the filter is implicitly imposed by the computational grid, and the resulting subgrid-scale (SGS) stresses must be modeled in terms of grid-resolved quantities to close the governing equations.

The primary challenge in LES is to formulate a physically accurate closure model for the SGS stresses, and many models have been proposed (see [1] for a review). To date, however, no SGS model has been found that in a priori tests accurately produces values of \( \tau_{ij}(x, t) \) that ensure the correct space- and time-varying momentum and energy exchange between the resolved and subgrid scales at each location and time. This is crucial to the accuracy of LES since errors in the modeled \( \tau_{ij}(x, t) \) field propagate up through the resolved scales. This inverse error cascade causes the resolved fields to appear non-deterministic,\(^2\) and the generated LES solutions at best solve the Navier-Stokes equations in a statistical sense.\(^3\)

Here we present a fundamentally new autonomic approach to closing the LES equations that does not
require a predefined constitutive model of the subgrid stress tensor in terms of resolved-scale quantities. Instead, the approach allows the simulation itself to determine the best local relation between the subgrid stresses and all resolved state variables, and uses the resulting local relation to evaluate the local subgrid stresses. We express the local subgrid stresses, \(\tau_{ij}(x,t)\), in terms of the most general polynomial of all resolved state variables and their products at all points and all times. The resulting general relation involves a very large set of unknown coefficients that can vary from point-to-point and with time as the local subgrid stress dynamics adapts to Lagrangian variations in the turbulence state. Any of the coefficients are allowed to be set to zero in the optimization procedure, so there is no predefined turbulence model in the autonomic approach. In this most general form, no assumptions are made as to how the subgrid stresses are related to the resolved primitive variables in the LES, beyond the fundamental assumption underlying all LES models that the subgrid stresses are a function of resolved-scale quantities, characteristic time and length scales, and the temporal and spatial domains. Incorporating the entire spatial and temporal domains improves the ability of the autonomic closure to capture challenging nonequilibrium, nonlocal, and time lag effects.\(^4\)\(^6\)

The polynomial coefficients in the general closure relation can be found by posing an inverse modeling problem at a test filter scale where the subgrid stresses are known. Applying standard test filters to the resolved fields yields a coarser field with known subgrid stresses. The primitive variables are also known at the test scale, and therefore optimal coefficients can be determined. Inverse modeling techniques such as regularization and sampling can be used to control the stability and computational cost of the solution. The resulting coefficients represent the best possible local relationship between resolved primitive variables and subgrid stresses. The coefficients can be thought of as representing both linear combinations of terms in the polynomial expansion and as finite difference coefficients approximating gradients. This results in a dynamic optimal constitutive relationship that allows enormous flexibility in accounting for different physical effects. As long as the test and LES scales are within the inertial range, the relationship between resolved quantities and subgrid stresses is approximately scale invariant and coefficients optimized at the test scale can be applied at the LES scale with appropriate rescaling of characteristic time and length scales.

This new closure approach is fully autonomic in the sense that it allows an LES to find, by itself, the optimal relation between local subgrid stresses at each point and time and all possible resolved quantities. The concept of relating subgrid stresses to resolved primitive variables is inherent in the whole notion of LES but, unlike traditional closure models, the present approach is essentially model-free in that it does not presume any specific constitutive relation between subgrid stresses and resolved scale physical quantities such as strain rates, rotation rates, or other quantities that appear in conventional SGS modeling. The only restriction on this new closure approach is that the turbulence should be scale-similar near the filter scale, since this is what allows the local set of optimal coefficients in the fully adaptive general relation between subgrid stresses and resolved state variables to be applied at the filter scale.

The present paper is organized as follows: relevant background is provided in Section II, the autonomic closure is outlined in Section III, Section IV provides initial a priori results using data from direct numerical simulations (DNS), and Section V provides a summary and an outline for future work.

## II. Relevant Background

### A. Low Pass Filtering the Navier Stokes Equations

In traditional LES, the Navier-Stokes equations are coarse-grained by filtering them to achieve scale separation between resolved and sub-filter scales. Ideally, the filter scale is in the scale-similar inertial range so that inertial-range scalings and scale-similarity concepts can be used in modeling the subgrid stress to achieve closure of the resulting LES equations. Conceptually, the scale separation is achieved by convolving the true velocity vector with a filter kernel \(G_{\Delta_{\text{LES}}}\), where \(\Delta_{\text{LES}}\) is the LES filter scale, giving the resulting filtered velocity field \(\tilde{u}\) as

\[
\tilde{u}(x,t) = G_{\Delta_{\text{LES}}} \ast u(x,t) = \int u(x',t') G_{\Delta_{\text{LES}}} (x - x',t - t') d^3x'dt',
\]

where \(\ast\) denotes the convolution operator. In practice, the convolution is often done implicitly when discretizing onto a numerical grid, resulting in a less well-defined kernel and filter scale, as well as changing subfilter stresses into subgrid stresses.

Filtering the Navier-Stokes equations with the convolution operator in Eq. (1) results in governing equations for \(\tilde{u}(x,t)\) that resemble the original equations, but with additional source terms that arise from
commutation errors between the scale separation operator $G_{\Delta,LES}$, the tensor or outer product operator, and time or space derivatives. Making the common assumptions that the filter $G_{\Delta,LES}$ is linear, preserves constants, and commutes with time and space derivatives, the incompressible LES equations are

$$\frac{\partial}{\partial x_i} \tilde{u}_i = 0, \quad \frac{\partial}{\partial t} \tilde{u}_i + \frac{\partial}{\partial x_j} (\tilde{u}_j \tilde{u}_i) + \frac{\partial}{\partial x_i} \tilde{p} - \nu \frac{\partial^2 \tilde{u}_i}{\partial x_j^2} = - \frac{\partial}{\partial x_j} \tau_{ij},$$

where $\tau_{ij} = \tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j$ represents the unclosed subfilter-scale stress due to the commutation error between convolution and tensor products and the density has been absorbed into the pressure. The filtered quantities $\tilde{u}_i$ and $\tilde{p}$ are solved on a computational mesh with grid size $h$, resulting in the resolved filtered fields $\tilde{u}_i^h$ and $\tilde{p}^h$. The grid scale is typically the filter scale $\Delta$ or slightly finer, and as a result the subfilter-scale stresses are truncated by the discretization process, making them SGS stresses. The SGS stresses must be closed with a model based on quantities involving $\tilde{u}_i^h$ and $\tilde{p}^h$, which are denoted hereafter as simply $\tilde{u}_i$ and $\tilde{p}$.

### B. Prior LES Subgrid Scale Turbulence Models

A wide variety of LES SGS models have been proposed, typically invoking scale similarity,\(^7\) the gradient transport hypothesis,\(^8\) dynamic filtering,\(^9\) deconvolution,\(^10\) regularization,\(^11\) or other principles.\(^12\) Nearly all such models employ a specific constitutive relation between the SGS stress tensor and one or more resolved-scale physical quantities, such as the strain rate, vorticity, or other quantities derivable from the resolved velocity and pressure. For example, the widely-used Smagorinsky model\(^9\) assumes a constitutive relation in which the deviatoric SGS stress $\tau_{ij}^S$ is related to the resolved strain rate, $\bar{S}_{ij} = \frac{1}{2} (\partial \tilde{u}_i / \partial x_j + \partial \tilde{u}_j / \partial x_i)$ via a turbulent viscosity, $\nu_t$, as

$$\tau_{ij}^S = 2 \nu_t \bar{S}_{ij}. \quad (3)$$

On dimensional grounds, $\nu_t$ is typically related to the filter length scale $\Delta$ and the dissipation rate $\varepsilon$ as $\nu_t \sim \Delta^4/\varepsilon^{1/3}$. Further assuming that the turbulence is in equilibrium such that $\varepsilon = -P = \tau_{ij}^D \bar{S}_{ij}$ then gives

$$\nu_t = C_s \Delta^2 \left( 2 \bar{S}_{ij} \bar{S}_{ij} \right)^{1/2}, \quad (4)$$

where $C_s$ is the Smagorinsky constant. Taken together, Eqs. (3) and (4) provide a modeled constitutive equation for the SGS stress. A popular extension\(^13,14\) involves dynamically determining values for the Smagorinsky constant, using a scale-similarity approach in which the known subgrid stresses from a test filter applied to the resolved velocities are used to infer a local value for $C_s$. This approach is implemented in our a priori tests as a comparison case for the autonomic closure.

Even with the dynamic approach for determining $C_s$, Smagorinsky-type models do not accurately produce the local space- and time-varying momentum and energy exchange between resolved and subgrid scales. Such models are based on the gradient transport hypothesis and eddy viscosity formulation in Eqs. (3) and (4), both of which suffer from fundamental flaws.\(^15\) In particular, gradient transport models inherently assume that the eigenvectors of $\tau_{ij}^D$ are always precisely aligned with those of $\bar{S}_{ij}$, which typically is not the case,\(^16\) and they further assume that the production and dissipation of turbulent kinetic energy is in equilibrium everywhere. Other SGS models have attempted to improve on the Smagorinsky approach, using various algebraic, nonlinear, or mixed tensor diffusivity models to provide more complex constitutive relations for $\tau_{ij}^D$ in terms of resolved-scale quantities. Semi-adaptive forms, such as the Vreman model,\(^17\) have also been proposed, but to date no SGS model has been developed that provides an accurate representation for the local space- and time-varying momentum and energy exchange between the resolved and subgrid scales that is fundamental to the LES formulation.

### C. Testing Procedures for LES Subgrid Scale Models

The accuracy of any proposed SGS model can be assessed in two ways, as noted by Meneveau and Katz.\(^1\) The first approach, termed a priori testing, filters velocity and pressure fields from DNS to provide synthetic LES fields, along with exact results for the corresponding subgrid stress fields $\tau_{ij}(x, t)$. The modeled subgrid stress fields are then calculated from the synthetic LES fields and compared with the exact subgrid stress fields to determine how accurately the model captures the local momentum and energy exchange between the resolved and subgrid scales. The second approach, called a posteriori testing, implements the proposed SGS model in an LES code and compares resulting values for resolved-scale quantities in a test problem with...
corresponding experimental or DNS results for the same test problem. Such \textit{a posteriori} tests do not reveal how well a given SGS model captures precise details of the momentum and energy exchange between the resolved and subgrid fields, but do allow the resulting net effects on the resolved scales to be assessed.

In Section IV, we use \textit{a priori} testing to assess in precise detail how well the proposed autonomic closure approach, presented in Section III, is able to provide the correct subgrid stress fields $\tau_{ij}(x, t)$ using only the resolved velocity and pressure fields accessible in an LES.

### III. The Autonomic LES Subgrid-Scale Closure

The Autonomic LES closure (hereafter abbreviated as “ALES” closure) is based on the most general polynomial expression relating the local subgrid stress tensor to all resolved state variables and their products at all points and times in the flow. The polynomial coefficients reflect both linear combinations of the polynomial terms and finite difference weights approximating gradients of the terms. The coefficients are determined by solving an inverse modeling problem for known SGS stresses at a test filter scale. Various inverse modeling techniques such as regularization, sampling and truncation can be applied to ensure that the optimization process is stable and efficient. The closure approach is fully autonomic, since it allows an LES without any imposed SGS model to find, by itself, the optimal relation between the local subgrid stresses and all possible quantities that are derivable as linear or nonlinear combinations of the resolved velocity and pressure fields. In this section, the ALES closure is outlined in its most general form, the inverse modeling problem is developed, regularization and sampling techniques are demonstrated, and nuances of the scale projection from the test filter scale to the LES scale are discussed.

#### A. The Fundamental Closure Assumption

Fundamentally, the search for any subgrid-scale closure amounts to formulating a closed expression for $\tau_{ij}$ in terms of primitive state variables obtained from the solution of governing equations. For an incompressible flow governed by the LES equations in (2), the state variables are the resolved-scale velocities $\tilde{u}$, and pressure $\tilde{p}$, where the density has been absorbed in the pressure. Moreover, in order to account for nonlocal and nonequilibrium effects the form of the closure should not preclude the possibility that $\tau_{ij}$ at a particular point and time depends on primitive variables at other points and times. Additionally, characteristic time and length scales should be included in the closure to help enforce dimensional and scale consistency. The most general SGS closure can thus be written as

$$
\tau_{ij}(x, t) = \mathcal{F}[\tilde{u}(x', t'), \tilde{p}(x', t'), x', t', \mathcal{L}, \mathcal{T}],
$$

where $x'$ denotes the entire spatial domain, $t'$ denotes all times, $\mathcal{L}$ is a characteristic length scale (e.g., the filter width $\Delta$), and $\mathcal{T}$ is a characteristic time scale (e.g., the resolved strain rate magnitude). All prior SGS models assume some functional form for $\mathcal{F}$. By allowing any linear or nonlinear combination of the state variables to appear in the function $\mathcal{F}$, it is possible to represent a wide range of mathematical operations, including temporal and spatial derivatives, filters, multi-point differences, and multi-point products.

Taking $\mathcal{F}$ to be a polynomial in terms of linear and nonlinear combinations of $\tilde{u}$ and $\tilde{p}$ and using $\mathcal{L}$ and $\mathcal{T}$ to ensure the dimensional consistency of each term, we introduce the general relation

$$
\tau_{ij}(x, t) = \frac{\mathcal{L}^2}{T^2} \left[ \alpha_{ij} k_{1n1m1} \left( \frac{T}{\mathcal{L}^2} \tilde{v}_{k1n1m1} \right) + \beta_{ij} k_{1n1m1k2n2m2} \left( \frac{T^2}{\mathcal{L}^3} \tilde{v}_{k1n1m1} \tilde{v}_{k2n2m2} \right) + \gamma_{ij} k_{1n1m1k2n2m2k3n3m3} \left( \frac{T^3}{\mathcal{L}^4} \tilde{v}_{k1n1m1} \tilde{v}_{k2n2m2} \tilde{v}_{k3n3m3} \right) + \frac{T^4}{\mathcal{L}^4} (4\text{th order terms}) + \ldots \right],
$$

where $m = [1, M]$ spans all discrete time steps, $n = [1, N]$ spans all three-dimensional discrete spatial locations, $\tilde{v}_{knm} = [\tilde{u}_3(x_n, t_m), \tilde{u}_2(x_n, t_m), \tilde{u}_3(x_n, t_m), \tilde{p}(x_n, t_m)]$ with $k = [1, 4]$, and summation is implied over repeated indices. The $k$, $n$, and $m$ indices are assumed to be vectorized such that the superscript indices on $\alpha$, $\beta$, and $\gamma$ denote position in a single dimension of these third order matrices.

#### B. Finding ALES Coefficients

The general relation for $\tau_{ij}$ in Eq. (6) introduces a large number of coefficients in the $\alpha$, $\beta$, $\gamma$, and higher order matrices. Since each of these matrices are third order, they can be concatenated along the vectorized...
superscript dimension to give a single matrix of ALES coefficients, denoted $\phi$. These coefficients will be found using inverse modeling and optimization techniques, which are the key steps in the ALES approach. This section introduces an objective function based on test filtering that quantifies error in the ALES model and can be used to drive the optimization process. We then invoke a scale similarity argument to apply ALES coefficients obtained using a test filter at the LES scale. Finally, the ALES closure is posed as an inverse modeling problem, and regularization and sampling techniques are applied.

1. Defining an Objective Function Via Test Filtering

We introduce a test filter scale, $\Delta_1$, that is larger than the LES filter scale, $\Delta_{LES}$, and characterizes an additional filtering operation, $G_{\Delta_1}$. This new filter defines the test filtered velocity field given by

$$\hat{u}(x,t) = G_{\Delta_1} \ast u(x,t) = \int u(x',t') G_{\Delta_1}(x-x',t-t') \, dx'dt'. \quad (7)$$

For simplicity, we take both $G_{\Delta_1}$ and $G_{\Delta_{LES}}$ to be spectrally sharp filters that are exact projection operators such that $\hat{u} = \hat{\hat{u}}$. Additionally, we define scale-specific SGS stresses $\tau_{ij}^{\Delta_{LES}} = \hat{u}_i \hat{u}_j - \bar{u}_i \bar{u}_j$ and $\tau_{ij}^{\Delta_1} = \hat{\hat{u}}_i \hat{\hat{u}}_j - \hat{\bar{u}}_i \hat{\bar{u}}_j$, where $\tau_{ij} \equiv \tau_{ij}^{\Delta_{LES}}$ is required for closure of the governing LES equations. Test filtering the LES field $\hat{u}(x,t)$ with $G_{\Delta_1}$ results in known values for the $\tau_{ij}^{\Delta_1}(x,t)$ and $\hat{u}(x,t)$ fields. This is sufficient to define an objective function $J(\hat{\hat{u}}, \hat{\bar{u}}, \phi)$ that measures error in the ALES model results for $\tau_{ij}^{\Delta_1}(x,t)$ as

$$J(\hat{\hat{u}}, \hat{\bar{u}}, \phi) = \|\tau_{ij}^{\Delta_1}(x,t) - \tau_{ij, ALES}^{\Delta_{LES}}(x,t; \hat{\hat{u}}, \hat{\bar{u}}, \phi)\|^2, \quad (8)$$

where $\phi$ is the set of ALES coefficients, $\tau_{ij, ALES}^{\Delta_{LES}}(x,t; \hat{\hat{u}}, \hat{\bar{u}}, \phi)$ represents the modeled stresses at scale $\Delta_1$ given by Eq. (6), and $\| \cdot \|$ denotes the $\ell^2$ norm over all time, space, and $ij$ components. The $\phi$ matrix that minimizes the objective function $J(\hat{\hat{u}}, \hat{\bar{u}}, \phi)$ provides the optimal local relation between $\tau_{ij}^{\Delta_1}(x,t)$ and linear and nonlinear combinations of $\hat{u}(x,t)$ and $\hat{\bar{u}}(x,t)$ as expressed generally by Eq. (6). Since any coefficient in $\phi$ can be found to be zero during the optimization for different flows or geometries, there is fundamentally no predefined turbulence model or constitutive equation in this autonomic approach.

2. Scale Projection to the LES Scale

As long as $\Delta_1$ and $\Delta_{LES}$ are both in the (approximately) scale-similar inertial range and the convolution filters are spectrally sharp, the functional relationship $F$ from Eq. (5) and expanded in Eq. (6) relating filtered quantities and SGS stresses should be constant at both scales due to scale invariance in the inertial range. The ALES coefficients that parameterize $F$ must then also be scale invariant throughout the inertial range as long as the filtering operator is only changing by the wavenumber of the cutoff. Consequently, we use the ALES coefficients optimized at $\Delta_1$ in our ALES expression for $\tau_{ij} = \tau_{ij, ALES}^{\Delta_1}$. Although the coefficients parameterizing $F$ are scale invariant, the actual SGS stresses themselves change in size and magnitude as the wavenumber of the filter cutoff changes. We account for this by making our characteristic time and length scales $T$ and $L$ scale-specific. We use $L_{\Delta_1} = \Delta_1$ and $T_{\Delta_1} = (2\tilde{S}_{ij}\tilde{S}_{ij})^{-1/2}$ in the optimization at our test scale, and $L_{\Delta_{LES}} = \Delta_{LES}$ and $T_{\Delta_{LES}} = (2\tilde{S}_{ij}\tilde{S}_{ij})^{-1/2}$ at the LES scale. This allows the ALES results for $\tau_{ij, ALES}^{\Delta_{LES}}$ to reflect the changes in intensity and scale of the SGS stresses when transitioning from $\Delta_1$ to $\Delta_{LES}$. Furthermore, we apply the coefficients to quantities separated by a normalized length scale. In practice, this means that any stencil applied as part of a spatial truncation must have its grid point spacing nondimensionalized by the filter length scale.

This test filtering and scale similarity approach is a crucial step in making this closure autonomic. No previous DNS simulations, training data, or user specified parameters are required. Instead, the approach leverages the scale-similar properties of the filtering process to create a field of known SGS stresses corresponding to known filtered velocities. Because of the scale-invariant properties of the relationship $F$, we are able to apply the test filter-optimized coefficients at our LES scale. In this way, the predicted ALES SGS stress fields are determined through a scale invariant functional relationship that incorporates scale-specific characteristic time and length scales. This makes the ALES approach fully autonomous and complete.
3. Inverse Modeling Problem for Optimal Coefficients

The ALES optimization process can be represented more generally as a discrete inverse modeling problem of the form

\[ \mathbf{Gm} = \mathbf{d}, \]

(9)

where \( \mathbf{d} \) is a vector of observations or data to be fit, \( \mathbf{G} \) is a model or operator representing a physical system, and \( \mathbf{m} \) is a vector of model parameters (the “model solution” in inverse modeling parlance) that must be determined. Minimizing the objective function \( J(\hat{\mathbf{u}}, \hat{\mathbf{p}}, \phi) \) in Eq. (8) can then be posed as a discrete least squares problem of the form

\[ \min_J \parallel \mathbf{d} - \mathbf{Gm} \parallel^2, \]

(10)

where \( \mathbf{J} \) is a quantity to be minimized, \( \mathbf{d} \) is an \( n \times 1 \) vector of known SGS stresses sampled from \( \tau_{ij}^\Delta (x, t) \), \( \mathbf{G} \) is an \( m \times n \) matrix whose rows represent the polynomial terms in \( F \) evaluated at each point where \( \tau_{ij}^\Delta (x, t) \) is sampled, and \( \mathbf{m} \) is an \( m \times 1 \) vector containing the ALES \( \phi \) coefficients in vectorized form.

Posing this as an inverse modeling problem is a powerful way to reveal many insights about the optimization process. First, the cost of the optimization process is driven by the size of the matrix \( \mathbf{G} \). The width, \( m \), of \( \mathbf{G} \) is determined by any truncations applied to Eq. (6), for example truncating to 2\textsuperscript{nd} order in velocity, a final timestep, and/or a local spatial stencil. The height, \( n \), is determined by the number of samples taken of \( \tau_{ij}^\Delta \). This sparse sampling reduces the computation cost, but also ensures that the observations are separated by at least a turbulent length scale and are therefore statistically independent. The rank of \( \mathbf{G} \) reveals how closely a solution vector \( \mathbf{m} \) can match the observations \( \mathbf{d} \), and the conditioning number of \( \mathbf{G} \) determines how stable the solution \( \mathbf{m} \) is when there is noise in the observations. Finally, the general inverse modeling form is also amenable to a statistical viewpoint, which can be useful for data assimilation, and regularization, which can improve stability and is discussed in the next section.

C. Regularizing the Inverse Problem

Inverse modeling problems are typically ill-posed due to the ill-conditioning of \( \mathbf{G} \) and therefore exhibit extreme sensitivity to changes in the observation data. As a result, noise or small variations in the test filtered SGS stresses in \( \mathbf{d} \) can result in large changes in the inverse solution \( \mathbf{m} \). This instability can be seen in the generalized inverse solution \( \mathbf{m}_i \) based on the Moore-Penrose pseudoinverses of \( \mathbf{G} \), given by

\[ \mathbf{m}_i = \mathbf{V}_p \Sigma_p^{-1} \mathbf{U}_p^T \mathbf{d} = \sum_{i=1}^p \frac{\mathbf{U}_p^T \mathbf{d}}{s_i} \mathbf{V}_i, \]

(11)

where \( \mathbf{G}^\dagger \) is the pseudoinverse, \( s_i \) are the singular values of \( \mathbf{G} \), the subscript \( p \) refers to the compact form of the singular value decomposition of \( \mathbf{G} \) with \( p \) nonzero singular values, and the subscript \( i \) referring to the \( i \)th column of \( \mathbf{U} \) or \( \mathbf{V} \). The columns of \( \mathbf{U} \) form a basis spanning the data space and the columns of \( \mathbf{V} \) form a basis spanning the model space. The inner product of the data space basis vector \( \mathbf{U}_i \) and the data vector \( \mathbf{d} \) yields a scalar weighting factor for the model space basis vector \( \mathbf{V}_i \). The model space basis vectors corresponding to small singular values are typically highly oscillatory and noisy while the basis vectors for large singular values are typically smooth. Random noise in the observations will \( \mathbf{d} \) likely have a component in the direction \( \mathbf{U}_i \) corresponding to a very small \( s_i \) singular value. As a result, that \( \mathbf{V}_i \) model space basis vector will dominate the solution \( \mathbf{m}_i \) and amplify the noise.

Instability in the inverse modeling solution is undesirable because the solution will reflect noise in the data rather than underlying physics and is often addressed with some form of regularization. Regularization techniques add additional information to prevent overfitting and represent a tradeoff between solution variance and error or bias in the fit. Common regularization techniques include augmenting the objective function with a weighted \( \ell^1 \) or \( \ell^2 \) norm of \( \mathbf{m} \) that penalizes large model parameter values, resulting in a new objective function \( \mathbf{L} = \mathbf{J} + \alpha \parallel \mathbf{m} \parallel \). The \( \ell^2 \) norm is computationally attractive because it is linear, whereas the \( \ell^1 \) norm is piecewise linear but selects a sparse solution. Another common regularization technique is Tikhonov Regularization which uses the new objective function

\[ \mathbf{L} = \mathbf{J} + \alpha \parallel \Gamma \mathbf{m} \parallel \]

(12)

where \( \Gamma \) can be the identity matrix to penalize solution norms or a finite difference matrix to penalize variation in the solution parameters.
In this study we employ a third category of regularization techniques for generalized inverse modeling solutions, the truncated singular value decomposition (TSVD). In the TSVD regularization we truncate the summation in Equation 11 at \( p' < p \), resulting in the TSVD solution

\[
m'_i = \sum_{i=1}^{p'} \frac{U_i^T d}{s_i} v_i. \tag{13}
\]

We choose \( p' \) based on the discrete Picard condition\(^{18}\) which requires that the numerator \( U_i^T d \) decay to 0 faster than the denominator \( s_i \) in Eq. (11). This process reduces the number of model space basis vectors used in \( m' \), but avoids instabilities due to small singular values. Put another way, this TSVD procedure provides an optimal way to truncate the general ALES expression based on the numerical properties of its discretized inverse modeling form. This also accelerates the optimization process since \( G^† \) can be found once and used repeatedly in finding \( m_i \) for each unique SGS stress component.

### IV. A Priori Testing of the ALES Closure

The ALES closure is evaluating here using a priori testing on DNS of homogeneous isotropic turbulence (HIT) and homogeneous sheared turbulence (HST). A priori testing is a necessary but not sufficient step in determining whether the closure will succeed in a forward a posteriori test. We use de-aliased \( 256 \times 256 \times 256 \) pseudospectral DNS results from a previously published and validated study\(^{19}\) and apply spectrally sharp filters at \( \Delta_{LES} \) and \( \Delta_1 \) to synthetically generate the LES and test filtered fields. With these filtered fields and the true DNS fields, the exact SGS stresses can be calculated at any scale and used to evaluate new turbulence models. The ALES results at \( \Delta_{LES} \) are compared to the exact SGS field and to the Dynamic Smagorinsky model from Lilly,\(^{13}\) which is a commonly used turbulence model that also employs a test filter and least squares optimization. We first present HIT and HST results for the least squares optimal ALES coefficients without regularization and then discuss the effects of a TSVD regularization.

#### A. Homogeneous Isotropic Turbulence Results

To demonstrate a minimal working example of the ALES closure, we truncate Eq. (6) to only include 1st and 2nd order terms, neglect the pressure field, consider only the final timestep, and limit the spatial extent to a \( 3 \times 3 \times 3 \) stencil around the sampling location. The physical separation between stencil points is normalized by the filter length scale. Furthermore, we sample \( \tau^\Delta_{ij} \) at every 10th point when creating \( d \), set \( \Delta_1 = 2\Delta_{LES} \), and seek a single solution vector \( m \) for each unique SGS stress component that is optimal over the entire flow domain. One could find an optimal \( m \) at each location for better accuracy in \( \tau^\Delta_{ij} \), but the inverse problem would be underdetermined. Furthermore, this misses the chance to discover any universality in the turbulent relationship \( F \) by seeking a single optimal \( m \) for the entire simulation.

The initial a priori tests are performed without any regularization and determine optimal coefficient matrices \( \alpha \) and \( \beta \) at the test filter scale using the relation

\[
\tau^\Delta_{ij}(x, t) = \frac{L^2}{T^2} \left[ T \sum_{k_1=1}^{3} \sum_{n_1=1}^{27} \alpha_{ij}^{k_1 n_1} \hat{v}_{k_1 n_1} + \frac{T^2}{L^2} \frac{1}{T} \sum_{k_1=1}^{3} \sum_{n_1=1}^{27} \sum_{n_2=1}^{3} \beta_{ij}^{k_1 n_1 k_2 n_2} \hat{v}_{k_1 n_1} \hat{v}_{k_2 n_2} \right] \tag{14},
\]

where the summation of terms has been expressed explicitly for the purposes of clarity. Note also that the index \( t \) has been used to denote the single temporal snapshot at which the initial testing has been performed. The optimal ALES coefficients are found at \( \Delta_1 \) by solving the discrete least squares minimization in Eq. (10) for the truncated expression in Eq. (14) using a QR decomposition. The size of the \( G \) matrix created by this sampling frequency is \( 17576 \times 3403 \). The optimal coefficients are then applied at every location in the domain at \( \Delta_{LES} \) using the relation

\[
\tau_{ij}(x, t) = \tau^\Delta_{ij}(x, t) \frac{L^2}{T^2} \left[ \frac{L^2}{T^2} \sum_{k_1=1}^{3} \sum_{n_1=1}^{27} \alpha_{ij}^{k_1 n_1} \hat{v}_{k_1 n_1} + \frac{T^2}{L^2} \sum_{k_1=1}^{3} \sum_{n_1=1}^{27} \sum_{n_2=1}^{3} \beta_{ij}^{k_1 n_1 k_2 n_2} \hat{v}_{k_1 n_1} \hat{v}_{k_2 n_2} \right] \tag{15},
\]

where \( L \) and \( T \) are here calculated using quantities at \( \Delta_{LES} \) and the discrete spatial locations indexed by \( n_1 \) and \( n_2 \) have been rescaled based on the ratio \( \Delta_1/\Delta_{LES} = 2 \).
Figure 1: Velocity fields, true SGS fields, 2\textsuperscript{nd} order ALES predictions and Dynamic Smagorinsky predictions at the test filter scale $\Delta_1$ for three different components of the SGS stress field in homogeneous isotropic turbulence (HIT). As expected, ALES shows good agreement with the true SGS field at the scale where the coefficients were optimized.

Figure 2: Velocity fields, true SGS fields, 2\textsuperscript{nd} order ALES predictions and Dynamic Smagorinsky predictions at the LES filter scale $\Delta_{LES}$ for three different components of the SGS stress field in homogeneous isotropic turbulence (HIT). ALES performs remarkably well when applying the test-filter optimized coefficients directly at the LES scale.

Figure 1 shows the velocity fields $u_1$, $u_2$, and $u_3$ filtered at $\Delta_1$ as well as the corresponding true SGS stresses $\tau_{11}$, $\tau_{13}$, and $\tau_{23}$ calculated from the DNS results, the SGS stress predictions from the 2\textsuperscript{nd} order ALES implementation in Eq. (14), and predictions for the same SGS stress components from the Dynamic Smagorinsky model. Since $\Delta_1$ is the scale at which the ALES coefficients are optimized, the ALES closure does an excellent job of capturing the structure, location, and intensity of the SGS stresses. The true test...
of the ALES closure and the scale invariance of the ALES coefficients is shown in Figure 2, which shows the same velocity and SGS stress components as those in Figure 1 but at $\Delta_{LES}$ using Eq. (15). At $\Delta_{LES}$, the true SGS stress structures are noticeably smaller, sharper, and more intermittent than at the test filter scale, but the ALES closure is able to capture nearly all of these features. This agreement is remarkable considering the severe truncation applied in Eq. (15) and noting that for each SGS stress component every location in the 3D field uses the same set of ALES coefficients.

The accuracy of the ALES closure can be quantitatively assessed by considering maps of the SGS stress errors shown in Figure 3. The error is defined as $\epsilon_{ij}(x) = \tau_{ij}^{\Delta_{LES, True}} - \tau_{ij}^{\Delta_{LES, ALES}}$. As shown in Figure 3, the ALES errors are have few pronounced spatial features since the model correctly predicts the structure of the SGS stresses. The Dynamic Smagorinsky model, by contrast, has errors of the same size, intensity, and structural complexity as the true SGS field itself, indicating that it generates incorrect instantaneous local stresses even if the mean energy transfers appear correct. The combined probability density function (pdf) of all of the error fields is shown in Figure 4 for two different ALES truncations and the Dynamic Smagorinsky model. Here we calculate pdf’s of the entire scalar error field $\epsilon(i, j, x, t) = \epsilon_{ij}(x, t)$ that includes each of the tensorial components and all locations of $\epsilon_{ij}(x, t)$. Even a first order ALES truncation is superior to the Dynamic Smagorinsky model, suggesting that even more severe truncations than that used in Eq. (15) may be possible.

B. Homogeneous Sheared Turbulence Results

We perform the a priori analysis on HST results using the same ALES truncations as in Eqs. (14) and (15) and also apply the same stencil, sampling, and QR decomposition to find the ALES coefficients. We seek...
least squares optimal Dynamic Smagorinsky coefficients in planes of homogeneous shear instead of across the entire volume as in the HIT case. However, we still seek one set of ALES coefficients across the entire sheared flow, thus presenting a more difficult prediction challenge for the ALES closure. Figures 5 and 6 show that we again see excellent agreement between ALES and the true SGS stress fields at $\Delta_1$ and moderate agreement at $\Delta_{LES}$. The error maps in Figure 7 and error pdfs in Figure 8 again show a substantial improvement over the Dynamic Smagorinsky results. While the accuracy of ALES in HST is not quite as good as in HIT, it is nonetheless very impressive given that the ALES coefficients are optimized over the entire domain and not
Figure 7: Similar results as in Figure 3 but for homogeneous sheared turbulence (HST), showing error maps for 2nd order ALES (top row) and Dynamic Smagorinsky (bottom row) at $\Delta_{LES}$ for all unique components of the SGS stress tensor. Errors from the present ALES closure are again substantially smaller than those from the Dynamic Smagorinsky approach.

Figure 8: Similar results as in Figure 4 but for homogeneous sheared turbulence (HST), showing error probability density functions for 1st and 2nd order ALES closures and the Dynamic Smagorinsky model at both $\Delta_1$ (left) and $\Delta_{LES}$ (right).

in homogeneous planes as in the Dynamic Smagorinsky model. The Dynamic Smagorinsky model requires averaging across homogeneous directions, which constitutes 256 different least squares optimizations for each plane in the DNS results. The ALES approach still only requires one optimization step for the entire flow, suggesting it may be a more advantageous SGS closure in complex or inhomogeneous flows.

C. Truncated SVD Regularization

The pure least squares solutions implemented in the previous sections exhibit small scale noise in the HIT results and in some cases miss or overpredict SGS stresses in the HST results. Many of these errors can be attributed to overfitting the data at $\Delta_1$. To stabilize the solution, we implement the truncated singular value decomposition regularization scheme described by Eq. (13). We use the discrete Picard condition which requires that the numerator $U_i^T d$ in the generalized inverse solution $m_1^\dagger$ decay to 0 faster than the denominator $s_i$. Figure 9 shows plots of the ratio of these two terms for HIT and HST. The number of retained singular values, $p'$, corresponds to the number of singular values where the ratio $U_i^T d / s_i < 1$. This ensures that small singular values are not causing their corresponding oscillatory model space basis vectors to dominate. We set $p' = 500$ in both HIT and HST, which is about $1/7^{th}$ of the original 3403 nonzero singular values.

The TSVD approach allows us to calculate the truncated pseduoinverse $G^\dagger = V_{p'} \Sigma_{p'}^{-1} U_{p'}^T$ once, and then quickly find the TSVD model solution for each component of the SGS stresses with a simple matrix-vector multiplication $m_1 = G^\dagger d$. The ALES estimate of the SGS stresses is then given by the TSVD model solution...
and the full $G$ matrix as $\tau_{ij}^{\Delta_{LES}} = Gm_i$.

We find the most improvement with the TSVD approach in the HST tests. The $\ell^2$ norm of the error at $\Delta_{LES}$ is 94.97 when using the least squares solution without any regularization and 81.3 when using the TSVD approach and $p' = 500$. Conversely, with HIT we find an $\ell^2$ norm of the error at $\Delta_{LES}$ to be 2639.9 without regularization and 2545.4 when using the TSVD approach. This suggests that the HST ALES results are more prone to overfitting than the HIT flow realization. The regularization scheme slightly hurts the error at the test filter scale $\Delta_1$, but it avoids overfitting the model $m$ to noise in the SGS stress data and improves the performance at the LES scale $\Delta_{LES}$ where it matters most. Figure 10 shows reduced performance in the ALES fit at $\Delta_1$, however Figure 11 shows the improved ALES SGS field at $\Delta_{LES}$. This improvement is further demonstrated in the $\Delta_{LES}$ error maps in Figure 12 and the error PDF in Figure 13.

V. Summary and Discussion

Here we have presented a fundamentally new and highly promising autonomic approach to estimating the subgrid-scale stresses needed to achieve closure in large eddy simulations of turbulent flows. The approach is based on the most general of all possible relations between the local subgrid-stress tensor and all resolved-scale variables at all points and times in the flow. The present turbulence closure is fully adaptive, allowing the general relation between the subgrid stresses and the resolved-scale fields to change freely as the local turbulence state changes. Lack of comparable adaptivity in conventional subgrid-scale models, which are based on predefined constitutive for the subgrid stresses in terms of the resolved strain rate or other resolved-scale quantities, may be a key reason why such models have to date failed to give accurate results for the subgrid stresses $\tau_{ij}(x, t)$ needed to ensure correct local momentum and energy exchange between the resolved and subgrid scales in LES.

Results presented here from a priori tests of this autonomic closure approach in homogeneous isotropic and sheared turbulence show that the new approach provides highly accurate estimates for the subgrid stress fields $\tau_{ij}(x, t)$ using only the resolved-scale fields available in LES. This is true even for a stringent truncation to 2nd order velocity terms and a small $(3 \times 3 \times 3)$ stencil, which can only accommodate second-order central differences. The accuracy of these test results, even for this small stencil, suggests that the autonomic closure can be implemented in a computationally efficient manner in practical LES. Moreover, the stencil size can be increased if higher-order gradients of resolved-scale quantities are needed to accurately capture states of turbulence that may occur under strong nonequilibrium or other extreme conditions.

A. Recap of the Autonomic Closure Process

After demonstrating a priori the success of the ALES closure, it is useful to recap the key steps in the process. First, a fundamental closure assumption is made in Eq. (5) that the SGS stresses can be expressed as a function of known resolved filtered quantities. This assumption underlies all prior SGS models, and the polynomial expansion presented in Eq. (6) is the most general expression of this relationship. The polynomial expansion introduces a large number of ALES coefficients, which we solve for using an optimization and inverse modeling machinery. To drive the optimization we establish a cost function based on error in the ALES SGS stress predictions at a test filtered scale $\Delta_1$ where velocities and SGS stresses are known. We then assume that the functional form of $F$ in Eq. (5) should be scale invariant within the inertial range, and consequently the ALES coefficients derived at $\Delta_1$ should be applicable at $\Delta_{LES}$. This assumption is validated by the performance of the ALES model in correctly predicting the SGS stresses at $\Delta_{LES}$ using the coefficients from $\Delta_1$. We then pose the optimization at the test filter scale as an inverse modeling problem and show how regularization techniques can be applied to the generalized inverse solution for $m$. Least squares optimal and regularized solutions using a truncated singular value decomposition are applied to HIT and HST in a priori testing. We find that the 2nd order ALES implementation has approximately half the error of the Dynamic Smagorinsky model when measured by the $\ell^2$ norm of the error field. The TSVD regularization improves the performance of the ALES model at the $\Delta_{LES}$ scale by 3.6% in the HIT case and by 14.4% in the HST case, while also decreasing the total computational cost.

B. Additional Considerations

The autonomic closure leverages a number of concepts that are uncommon in prior SGS turbulence models. Specifically, the inverse modeling formulation and multi-scale optimization introduce new issues regarding
Figure 9: Results from TSVD regularization of the autonomic closure approach, showing discrete Picard condition for 2nd order ALES in homogeneous isotropic turbulence (HIT, top) and homogeneous sheared turbulence (HST, bottom).

Figure 10: Similar results as in Figure 5 for homogeneous sheared turbulence (HST), but for truncated SVD regularization of the autonomic closure. Note that modeled stresses from ALES at the test filter scale are slightly degraded due to the small set of model space basis vectors.
Figure 11: Similar results as in Figure 6 for homogeneous sheared turbulence (HST), but for truncated SVD regularization of the autonomic closure.

Figure 12: Similar results as in Figure 7 for homogeneous sheared turbulence (HST), but for truncated SVD regularization of the autonomic closure, showing error maps for 2\textsuperscript{nd} order ALES (top row) and Dynamic Smagorinsky (bottom row). Errors from truncated SVD regularization are now seen to be smaller than those in Figure 7, and are again substantially smaller than those from the Dynamic Smagorinsky approach.

Figure 13: Similar results as in Figure 8 but for homogeneous sheared turbulence (HST), showing error pdfs for 1\textsuperscript{st} and 2\textsuperscript{nd} order ALES closures and the Dynamic Smagorinsky model at both $\Delta_1$ (left) and $\Delta_{LES}$ (right). Note the reduction of errors in the truncated SVD regularization of 2\textsuperscript{nd}-order ALES closure.
convexity, regularization, and universality. While the new autonomic closure is more flexible and general than
prior models with predefined turbulent constitutive equations, its inherently dynamic and evolving nature
makes it difficult to evaluate common SGS modeling criteria such as Galilean invariance and realizability
since the ALES closure is not in tensor form. Furthermore, the autonomic closure has been developed
and tested using spectrally sharp filters where an exact scale separation can be imposed and the nuances
of subfilter versus subgrid scale information are minimized. Implementing the ALES general polynomial
expansion and optimization process is less clear cut when considering filters with broad spectral support.
When applying a Gaussian or box type filter some information about the subfilter scales is retained in the
resolved scales, making deconvolution-type SGS models advantageous. The best SGS modeling approach
for spectrally broad filters may involve a hybrid of deconvolution kernels and the autonomic optimization
process.

The inverse modeling formulation introduced here facilitates regularization of the solution, but introduces
a bias into the solution that increases error and clouds statistical confidence intervals of the ALES model
coefficients. However, the inverse modeling formation does facilitate a Bayesian approach to finding posterior
distributions of model coefficients. This approach is useful for forward simulations because a general prior
distribution of the values of \( m \) can be provided to initialize a simulation, which is then updated with
information from the test filtering and optimization process in a Bayesian manner. Furthermore, the discrete
inverse modeling form also lends itself to a variational or sequential data assimilation process that could
incorporate simulation or experimental data to improve the solution of the model parameters \( m \) and their
covariances.

C. Future Work

The initial a priori tests of a truncated ALES implementation are very promising. Despite limiting the
order, spatial, and temporal extent of the function \( F \), the ALES process does an excellent job of predicting
the SGS stresses at both the test filter scale and the LES scale when measured by error norms or qualita-
tive assessments of the SGS fields. The next step is to integrate the ALES closure into a forward model
simulation and perform a posteriori tests. Additional work characterizing the tradeoffs between truncation,
regularization, and computation cost will be performed in both a priori and a posteriori contexts.

Further testing is also needed to explore the effect of stencil size on the accuracy of this closure approach,
including extreme turbulence states that may require higher-order terms in the general closure relation
and larger stencils to accommodate them. The closure must also be tested in a posteriori simulations of
homogeneous turbulence, inhomogeneous free and wall-bounded turbulent shear flows, and finally in complex
turbulent flow simulations where a high degree of generality and autonomic adaptability may be needed to
enable accurate representation of the subgrid stresses. These tests are more representative of the flows found
in engineering applications where the ALES closure will ultimately be implemented.

Additionally, it may be possible to extend this autonomic closure approach to steady and unsteady
Reynolds averaged Navier-Stokes simulations. The corresponding Reynolds stresses would be similarly ex-
pressed via the most general of all possible relations in terms of the averaged velocities and pressure at all
points in the flow, leading to an analogous coefficient matrix \( \phi \). Applying the equivalent of a spatial test
filter to coarsen the resolution of the averaged fields might then allow an analogous approach as used here
to determine the coefficients in \( \phi \), and thereby provide a comparable model-free autonomic closure for the
Reynolds stresses.

References


American Institute of Aeronautics and Astronautics

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